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Numerical Computation of the Effective Quasistatic Permittivity for Isotropic Lattices of Complex Shaped Inclusions

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Abstract

A technique is presented for the accurate computation of the effective quasistatic permittivity of lattices containing particles with potentially complicated shape. This technique is based on the moment method for the computation of the electric dipole moments of the dielectric or conducting particles. Through proper homogenization of the lattice, a simple formula for the effective permittivity is given in terms of these particle dipole moments. Verification data is presented for lattices of dielectric spheres obtained with the *T*-matrix method. Results are shown for lattices of dielectric cubes. Mutual interaction between the edges and corners of such a lattice combine to reduce the effective permittivity to values near the lower Hashin-Shtrikman bound.

1. Introduction

The computation of the effective material constants for lattices of particles has in the past been restricted primarily to inclusions of canonical shape. For example, Rayleigh's approximate analysis considered round cylinders and spheres [1] and McPhedran, McKenzie and Derrick considered cubic lattices of spheres [2, 3]. Additionally, our recent work has produced solutions for multiphase lattices of spheres and round cylinders [4, 5]. One exception to this canonical shape rule is the work of Sareni, *et al.* who considered lattices of rods and disks, among other shaped particles [6, 7].

The objectives of this work are twofold. First, we present a methodology for the computation of the effective quasistatic permittivity for lattices of complex shaped particles. That is, particles with edges, corners or other complicated surface features such as those present on cubes (in 3-D lattices) and square cylinders (in 2-D lattices). This methodology is based on the moment method (MM) wherein a set of electric potential integral equations is solved for the infinite lattice and the electric dipole moments of the particles are computed. By properly homogenizing this lattice, we obtain an accurate effective permittivity that properly captures the scattering by the particles and their interactions.

The second primary objective of this work is to investigate the effect of the inclusion shape on the resulting effective permittivity. For example, to investigate the edge effects and the mutual interaction between particles with sharply defined edges and the resulting effective permittivity.

2. Integral Equation Solution for the Dipole Moments

The first step in the computation of the effective quasistatic permittivity for lattices of complex shaped particles is the accurate determination of the electric dipole moments of the particles when the lattice is illuminated by a uniform (but otherwise arbitrary) electric field. We have chosen to use the

MM for these calculations since the particles may not be of canonical shape. Following the surface equivalence theorem, exterior and interior equivalent problems are constructed using equivalent single (ρ_s) and double (τ) layers of charge density [8, 9]. Shown in Fig. 1, for example, is a portion of the original lattice as well as the exterior and interior equivalent problems.

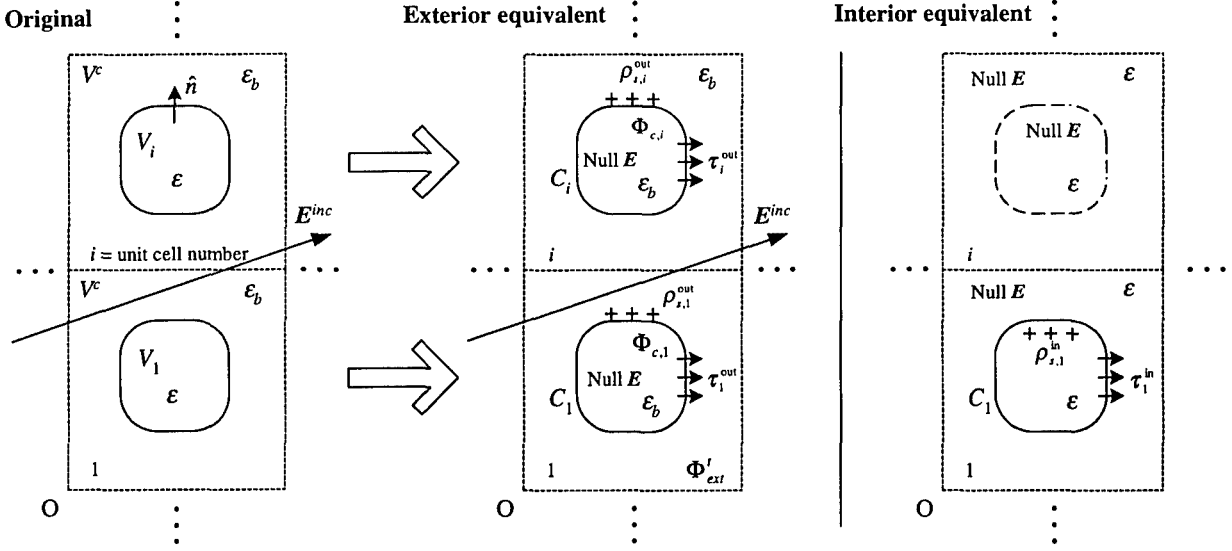


Figure 1 Geometry of the original and exterior equivalent scattering problems.

The scattered scalar potentials produced by these two types of equivalent sources are

$$\Phi_1(\mathbf{r}|\varepsilon, \rho_s) = \frac{1}{4\pi\varepsilon} \iint_S \frac{\rho_s}{R} ds' \quad (1)$$

$$\Phi_2(\mathbf{r}|\varepsilon, \tau) = \frac{1}{4\pi\varepsilon} \iint_S \tau \cdot \nabla' \left(\frac{1}{R} \right) ds' \quad (2)$$

In our MM solution to this lattice problem, we expand the two types of charge in sets of coincident constant basis functions

$$\rho_s = \sum_{n=1}^N \alpha_n T_n(\mathbf{r}') \quad (3)$$

$$\tau = \sum_{n=1}^N \hat{n} \beta_n T_n(\mathbf{r}') \quad (4)$$

where T_n is the n^{th} flat triangular patch on the surface of the scatterer.

Using a simple point matching scheme and enforcing the proper boundary conditions in the exterior and interior equivalent problems [9], the following set of integral equations can be formed

$$-\frac{1}{4\pi\varepsilon_b} \sum_{n=1}^N \alpha_n \left(\sum_{i=1}^{\infty} \iint_{S_n} \frac{1}{R_{mn}} ds' \right) - \frac{1}{4\pi\varepsilon_b} \sum_{n=1}^N \beta_n \left(\sum_{i=1}^{\infty} \iint_{S_n} \hat{n} \cdot \nabla' \left(\frac{1}{R_{mn}} \right) ds' \right) - \Phi_{c,1} = \Phi^{\text{inc}}(\mathbf{r}_1) \quad (5)$$

$$-\frac{1}{4\pi\varepsilon} \sum_{n=1}^N \alpha_n \left(\iint_{S_n} \frac{1}{R_{mn}} ds' \right) - \frac{1}{4\pi\varepsilon_b} \sum_{n=1}^N \beta_n \left(\iint_{S_n} \hat{n} \cdot \nabla' \left(\frac{1}{R_{mn}} \right) ds' \right) = 0 \quad (6)$$

where the i summation is over all particles in the lattice and $\Phi_{c,1}$ is the constant and unknown potential of particle 1. The double layer of surface charge we are solving for has zero average value over the surface so we add the constraint

$$\sum_{n=1}^N \beta_n A_n = 0 \quad (7)$$

In matrix form, Eqns. (5) through (7) can be expressed as

$$\begin{bmatrix} [Z_{11}]_{N \times N} & [Z_{12}]_{N \times N} & [1]_{N \times 1} \\ [Z_{21}]_{N \times N} & [Z_{22}]_{N \times N} & [0]_{N \times 1} \\ [0]_{1 \times N} & [A_n]_{1 \times N} & 0 \end{bmatrix} \begin{bmatrix} [\alpha]_{N \times 1} \\ [\beta]_{N \times 1} \\ -\Phi_{c,1} \end{bmatrix} = \begin{bmatrix} [\Phi^{inc}(r_1)]_{N \times 1} \\ [0]_{N \times 1} \\ 0 \end{bmatrix} \quad (8)$$

Once the matrix equation in (8) has been solved, the electric dipole moments of the particles can be computed as

$$p = \oint_{C_i} (\rho_s \rho' + \tau) ds' \quad (9)$$

In the case of isotropic lattices, the effective permittivity can be determined using the simple and accurate expression [4, 10]

$$\epsilon_{r,eff} = 1 + 3 \frac{p / (3\epsilon_0 E^{inc} V_c)}{1 - p / (3\epsilon_0 E^{inc} V_c)} \quad (10)$$

We reiterate that after following the methodology presented in this section, this $\epsilon_{r,eff}$ properly accounts for all scattering from (and mutual interactions between) particles that have possibly very complicated shape. A similar procedure has been developed for conducting 3-D particles as well as dielectric and conducting complex shaped 2-D cylinders [9, 11].

3. Results

In order to verify the accuracy of this technique, the effective permittivity of a simple cubic (SC) lattice of dielectric spheres with $\epsilon_r = 40$ was computed for varying volume fraction f . These results are shown in Fig. 2. This $\epsilon_{r,eff}$ compares well with $\epsilon_{r,eff}$ computed using our T -matrix solution [4]. These two results deviate by no more than 1% even at ultra-high volume fractions ($f > 0.5$).

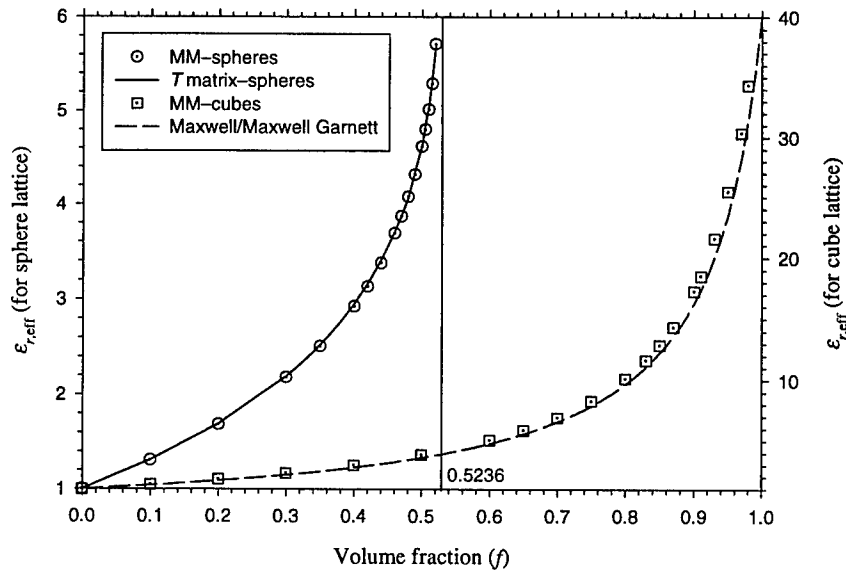


Figure 2 Computed $\epsilon_{r,eff}$ for SC lattices of dielectric spheres and dielectric cubes. In both cases the particles have $\epsilon_r = 40$. Notice that the two vertical axes have different scales.

Also shown in Fig. 2 is $\epsilon_{r,eff}$ for a SC lattice of dielectric cubes with $\epsilon_r = 40$. Unlike the sphere lattice, the maximal volume fraction for this lattice is 1. For most of these MM cube results, 1304 flat triangular cells were used to discretize the cubes and 27 unit cells were used to truncate the infinite lattice sums for the numerical calculations. For volume fractions $f > 0.95$, however, it was necessary to increase both the discretization and the number of unit cells (1890 and 125, respectively) to achieve less than 1% variation in the electric dipole moment of the dielectric cube.

While there is no accurate analytically based formula with which to compare these results for the lattice of dielectric cubes, we alternatively present the Maxwell/Maxwell Garnett (MG) predictions [12, Arts. 314 and 430]. Interestingly, it is apparent that the MM results for the cubes and the MG predictions are quite close (up to approximately 9% variation at $f = 0.98$). Even closer agreement has been observed for conducting square 2-D cylinders where the maximum variation is less than 0.4% at $f = 0.99$ [11].

The close agreement between the cube and MG results in Fig. 2 may appear at first glance to be the result of little mutual coupling between the cubes at high volume fraction. However, our investigations have shown that this is not the case [11]. Instead, the close agreement in these dielectric cube results (and other similarly shaped particles shown elsewhere [9, 11]) is likely the result of the large mutual interaction between the edges and corners of the particles. Interestingly, such interactions produce a reduction in the polarization of the particles with respect to the isolated case. Consequently, the effective permittivity of the lattice is reduced almost to the theoretically minimal amounts predicted by the lower bound of Hashin and Shtrikman [13, 14].

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